

10/569,159 Yong Chu 10-02-2007

\$%^STN;HighlightOn=;HighlightOff=;

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NEWS 2	JUL 02	LMEDLINE coverage updated
NEWS 3	JUL 02	SCISEARCH enhanced with complete author names
NEWS 4	JUL 02	CHEMCATS accession numbers revised
NEWS 5	JUL 02	CA/Caplus enhanced with utility model patents from China
NEWS 6	JUL 16	Caplus enhanced with French and German abstracts
NEWS 7	JUL 18	CA/Caplus patent coverage enhanced
NEWS 8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9	JUL 30	USGENE now available on STN
NEWS 10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 11	AUG 06	BEILSTEIN updated with new compounds
NEWS 12	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 13	AUG 13	CA/Caplus enhanced with additional kind codes for granted patents
NEWS 14	AUG 20	CA/Caplus enhanced with CAS indexing in pre-1907 records
NEWS 15	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 16	AUG 27	USPATOLD now available on STN
NEWS 17	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 18	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 19	SEP 13	FORIS renamed to SOFIS
NEWS 20	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 21	SEP 17	CA/Caplus enhanced with printed CA page images from 1967-1998
NEWS 22	SEP 17	Caplus coverage extended to include traditional medicine patents
NEWS 23	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 24	OCT 02	CA/Caplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS EXPRESS	19 SEPTEMBER 2007:	CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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0.21

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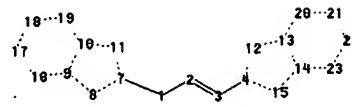
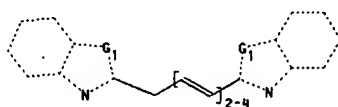
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

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=>

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chain nodes :
1  2  3
ring nodes :
4  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23
chain bonds :
1-2  1-7  2-3  3-4
ring bonds :
4-12  4-15  7-8  7-11  8-9  9-10  9-16  10-11  10-19  12-13  13-14  13-20  14-15
14-23  16-17  17-18  18-19  20-21  21-22  22-23
exact/norm bonds :
1-2  1-7  2-3  3-4  4-12  4-15  7-8  7-11  8-9  9-10  9-16  10-11  10-19  12-13
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G1:C,O,S,N,Se

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Match level :
1:CLASS  2:CLASS  3:CLASS  4:Atom  7:Atom  8:Atom  9:Atom  10:Atom  11:Atom
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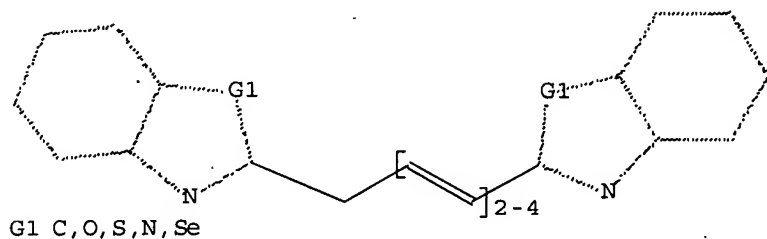
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 13:37:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 990 TO ITERATE

100.0% PROCESSED 990 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 17913 TO 21687

PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 full

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FULL SCREEN SEARCH COMPLETED - 20818 TO ITERATE

100.0% PROCESSED 20818 ITERATIONS
SEARCH TIME: 00.00.01

27 ANSWERS

L3 27 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

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172.31

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FILE LAST UPDATED: 1 Oct 2007 (20071001/ED)

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=> s l3

L4 10 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:477580 CAPLUS Full-text

DOCUMENT NUMBER: 113:77580

TITLE: Spectrophotometric studies of acid-base properties of cationic cyanine dyes

AUTHOR(S): Balog, I. S.; Kish, P. P.; Ishchenko, A. A.; Mushkalo, I. L.; Andrukh, V. A.

CORPORATE SOURCE: Uzhgorod State Univ., Uzhgorod, USSR

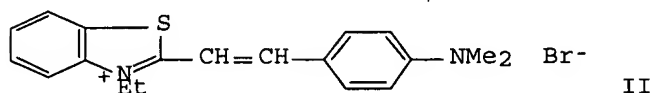
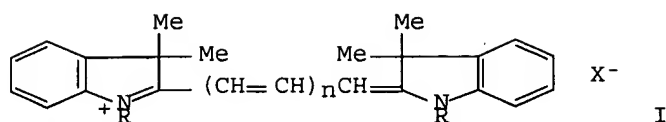
SOURCE: Zhurnal Analiticheskoi Khimii (1990), 45(3), 481-90

CODEN: ZAKHA8; ISSN: 0044-4502

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



AB The electronic absorption spectra and protonation and hydrolysis consts. of 12 cationic cyanine dyes, e.g., I (R = Me, CH₂CH₂OH, CH₂CH₂OAc; n = 1, 2, 3; X = Cl, Br) and II, were obtained. The dyes exist as reactive, singly charged forms over a wide acidity range. Charge distributions were calcd., and the protolysis mechanism was discussed.

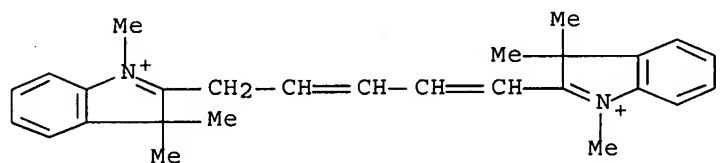
IT 128646-92-4 128646-93-5 128646-95-7

RL: PRP (Properties)

(UV spectrum of)

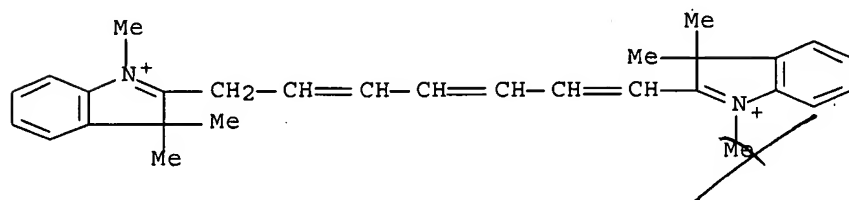
RN 128646-92-4 CAPLUS

CN 3H-Indolium, 2,2'-(1,3-pentadiene-1,5-diyl)bis[1,3,3-trimethyl- (9CI) (CA INDEX NAME)



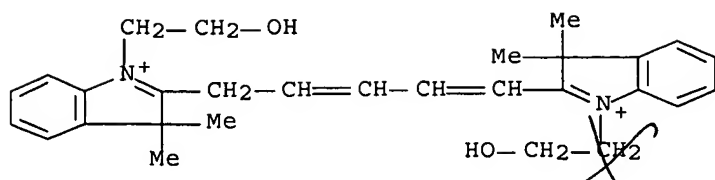
RN 128646-93-5 CAPLUS

CN 3H-Indolium, 2,2'-(1,3,5-heptatriene-1,7-diyl)bis[1,3,3-trimethyl- (9CI) (CA INDEX NAME)

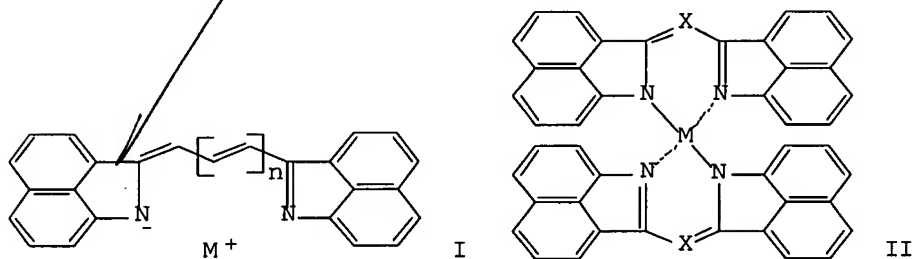


RN 128646-95-7 CAPLUS

CN 3H-Indolium, 2,2'-(1,3-pentadiene-1,5-diyl)bis[1-(2-hydroxyethyl)-3,3-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:181375 CAPLUS Full-text
 DOCUMENT NUMBER: 112:181375
 TITLE: N,N-cyanines of a benzo[c,d]indole series and their anionic dyes
 AUTHOR(S): Vasilenko, N. P.; Maidannik, A. G.; Mikhailenko, F. A.
 CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
 SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1989), 55(7), 742-6
 CODEN: UKZHAU; ISSN: 0041-6045
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

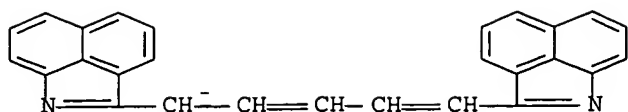


AB The cyanine dyes I ($M = \text{Li, Na, K}$; $n = 0, 1, 2$) and II ($X = \text{CH, N}$; $M = \text{Zn, Cu, Co, Ni}$) were prepd. and their spectra were studied with respect to structure. The absorption max. for I ($n = 1$) was little dependent on the nature of the counterion in THF or in DMSO, indicating the formation of ion pairs in the weakly polar THF. The form of the absorption curves for I anionic dyes, II complex dyes, and their cationic dye analogs was similar, indicating that the benz[c,d]indole chromophore system was responsible for the absorption in all cases.

IT 126667-25-2P 126667-26-3P 126667-27-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and spectral properties of)

RN 126667-25-2 CAPLUS

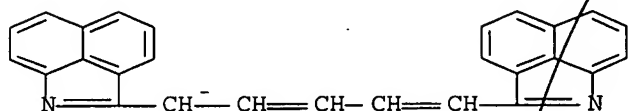
CN Benz[cd]indole, 2,2'-(1,3-pentadiene-1,5-diyl)bis-, ion(1-), lithium (9CI)
 (CA INDEX NAME)



● Li⁺

RN 126667-26-3 CAPLUS

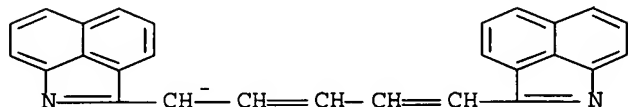
CN Benz[cd]indole, 2,2'-(1,3-pentadiene-1,5-diyl)bis-, ion(1-), sodium (9CI)
(CA INDEX NAME)



● Na⁺

RN 126667-27-4 CAPLUS

CN Benz[cd]indole, 2,2'-(1,3-pentadiene-1,5-diyl)bis-, ion(1-), potassium
(9CI) (CA INDEX NAME)



● K⁺

L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:38114 CAPLUS Full-text

DOCUMENT NUMBER: 112:38114

TITLE: Dimerization reactions of cyanine radical dications

AUTHOR(S): Parton, R. L.; Lenhard, J. R.

CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, 14650,
USA

SOURCE: Journal of Organic Chemistry (1990), 55(1), 49-57
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Radical dications formed during the one-electron oxidn. of representative cationic dicarbocyanine (pentamethine) dyes lacking alkyl substitution on the even-numbered carbon atoms of the methine chain underwent irreversible

dimerization in MeOH or MeCN soln. Deprotonation of the resultant UV-absorbing dimer gave a dicationic bis-dye with spectral properties similar to those of the parent dye. These bis-dyes were susceptible to further oxidn. via a reversible two-electron mechanism to yield a highly unsatd., cross-conjugated, tetracationic species. The chem. of radical dications derived from the one-electron oxidn. of carbocyanine (trimethine) dyes depended on the nature of the dye heterocycle as well as the degree of alkyl substitution in the methine chain. Some thiacarbo-cyanine radical dications irreversibly dimerized and gave products analogous to those obsd. for dicarbocyanines. A persistent radical dication was obtained by the one-electron oxidn. of an indolocarbocyanine and a chain-substituted thiacarbo-cyanine dye.

IT 123811-94-9P 123812-04-4P 123812-06-6P

123834-26-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectral properties of)

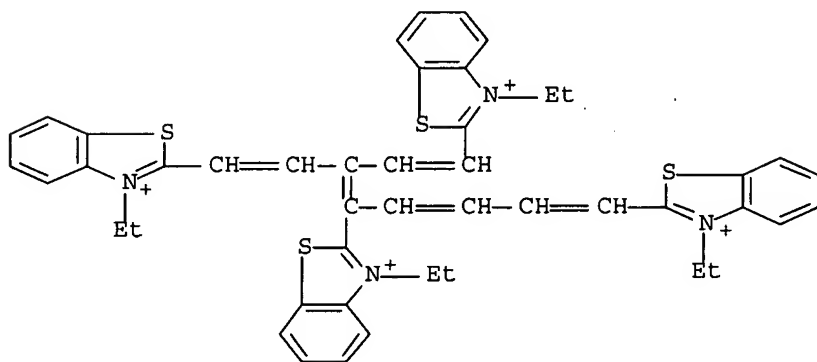
RN 123811-94-9 CAPLUS

CN Benzothiazolium, 2,2',2''-[3-[2-(3-ethylbenzothiazolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[3-ethyl-,
tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

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CRN 123811-93-8

CMF C46 H44 N4 S4

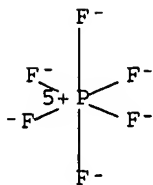


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CRN 16919-18-9

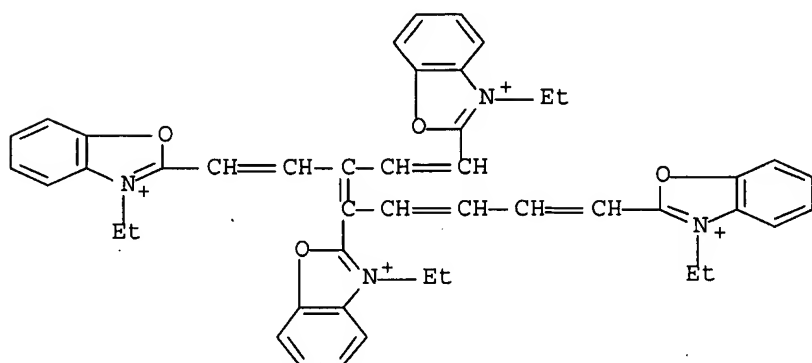
CMF F6 P

CCI CCS



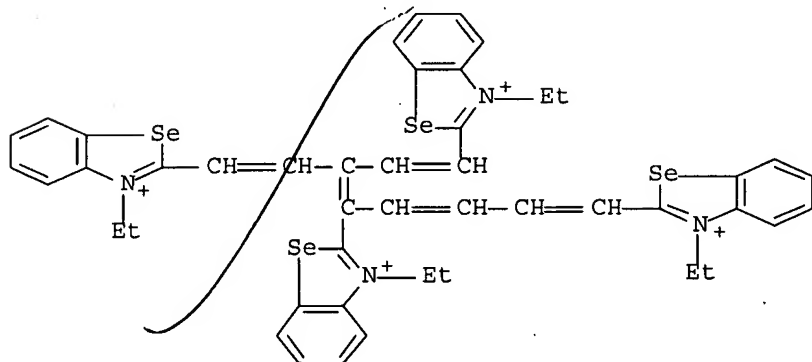
RN 123812-04-4 CAPLUS

CN Benzoxazolium, 2,2',2''-[3-[2-(3-ethylbenzoxazolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[3-ethyl- (9CI) (CA INDEX NAME)



RN 123812-06-6 CAPLUS

CN Benzoselenazolium, 2,2',2''-[3-[2-(3-ethylbenzoselenazolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[3-ethyl- (9CI) (CA INDEX NAME)



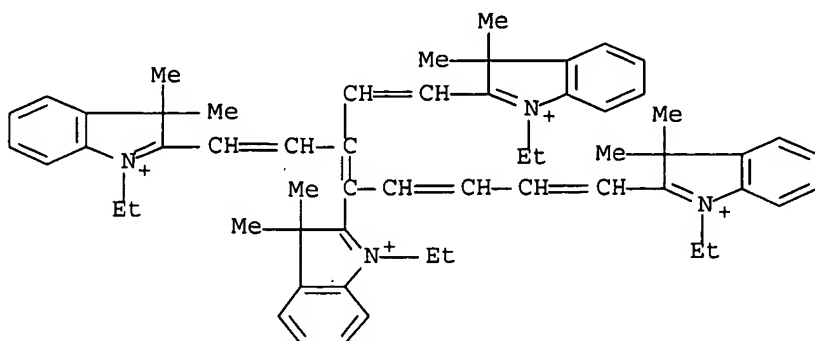
RN 123834-26-4 CAPLUS

CN 3H-Indolium, 2,2',2''-[3-[2-(1-ethyl-3,3-dimethyl-3H-indolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[1-ethyl-3,3-dimethyl-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 123834-25-3

CMF C58 H68 N4

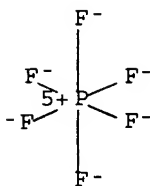


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

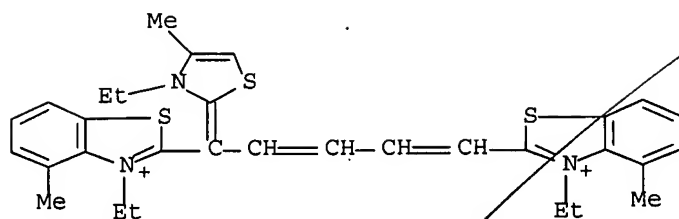


L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1977:185307 CAPLUS Full-text
 DOCUMENT NUMBER: 86:185307
 TITLE: Thin-layer chromatography of some cyanine dyes
 AUTHOR(S): Kues, H. A.; Teague, C. E.
 CORPORATE SOURCE: Appl. Phys. Lab., Johns Hopkins Univ., Laurel, MD, USA
 SOURCE: Journal of Chromatography (1977), 135(1), 221-5
 CODEN: JOCRAM; ISSN: 0021-9673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Various thin-layer chromatog. methods, as described by E. Stahl (1969), were tested on different subgroups of cyanine dyes, and RF values and dye purities were detd. Chromatog. was performed on silica gel sheets (100-.mu.m coating) and Al-backed silica gel sheets (250 .mu.m) with detection by white or UV light. The best results were obtained with the solvent systems 100% MeOH and PrOH-HCO2H (80:20). The 2 silica gel coatings, although showing some differences in a few cases, produced good reproducibilities.
 IT 60683-97-8
 RL: ANT (Analyte); ANST (Analytical study)
 (chromatog. of, thin-layer, purity in relation to)
 RN 60683-97-8 CAPLUS
 CN Benzothiazolium, 2,2'-[5-(3-ethyl-4-methyl-2(3H)-thiazolylydene)-1,3-pentadiene-1,5-diyl]bis[3-ethyl-4-methyl-, bis(ethyl sulfate) (9CI) (CA INDEX NAME)

CM 1

CRN 60683-96-7

CMF C31 H35 N3 S3



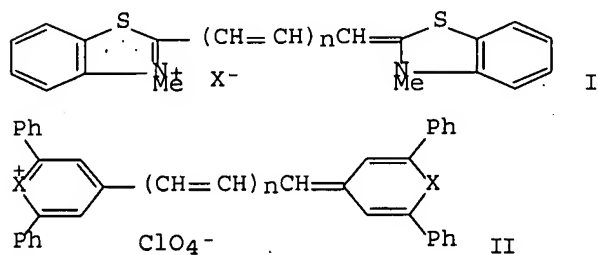
CM 2

CRN 48028-76-8

CMF C2 H5 O4 S

Et-O-SO₃⁻

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:107984 CAPLUS Full-text
DOCUMENT NUMBER: 86:107984
TITLE: Direction of polymethine dye protonation
AUTHOR(S): Tolmachev, A. I.; Kornilov, M. Yu.; Karaban, E. F.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Teoreticheskaya i Eksperimental'naya Khimiya (1976),
12(6), 817-21
CODEN: TEKHA4; ISSN: 0497-2627
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

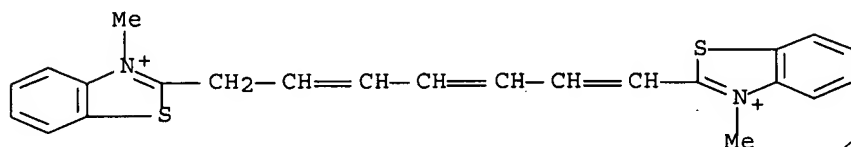


AB The UV and visible spectra and ¹H NMR spectra of CF₃CO₂H solns. of cyanine homologs I (n = 0-3, X = Cl, iodine) and II (n = 0-3; X = O, S) and of model compds. showed that protonation occurred at the CH adjacent to the heterocyclic ring.

IT 62077-45-6
 RL: PRP (Properties)
 (NMR and UV and visible spectra of)

RN 62077-45-6 CAPLUS

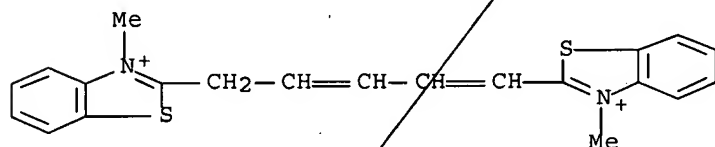
CN Benzothiazolium, 2,2'-(1,3,5-heptatriene-1,7-diyl)bis[3-methyl- (9CI) (CA INDEX NAME)



IT 62077-44-5
 RL: PRP (Properties)
 (NMR and UV spectra of)

RN 62077-44-5 CAPLUS

CN Benzothiazolium, 2,2'-(1,3-pentadiene-1,5-diyl)bis[3-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:572360 CAPLUS Full-text

DOCUMENT NUMBER: 85:172360

TITLE: Dyes can be deadly

AUTHOR(S): Kues, Henry A.; Luty, Gerard A.

CORPORATE SOURCE: Appl. Phys. Lab., Johns Hopkins Univ., Baltimore, MD, USA

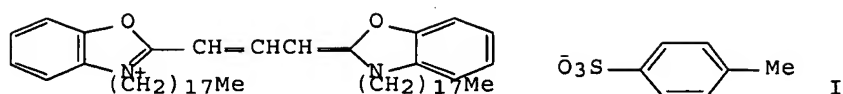
SOURCE: Laser Focus (Newton, Massachusetts) (1975), 11(5), 59-61

CODEN: LAFOAK; ISSN: 0023-8589

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Of various dyes tested, cyanine and carbocyanine compds. were the most toxic as evidenced by the LD100 value and survival time in mice after injection into the abdominal cavities. The 24-hr LD100 value of 3,3'-dioctadecyl-2,2'-oxacarbocyanine p-toluenesulfonate (I) [60711-74-2] was 5 mg/kg.

IT 60683-97-8

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of)

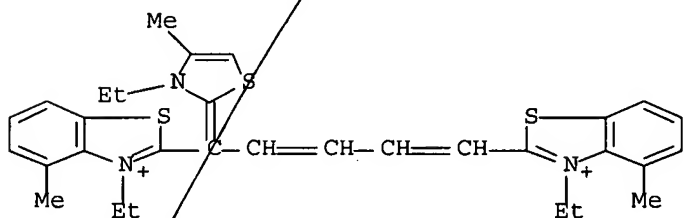
RN 60683-97-8 CAPLUS

CN Benzothiazolium, 2,2'-[5-(3-ethyl-4-methyl-2(3H)-thiazolylidene)-1,3-pentadiene-1,5-diyl]bis[3-ethyl-4-methyl-, bis(ethyl sulfate) (9CI) (CA INDEX NAME)

CM 1

CRN 60683-96-7

CMF C31 H35 N3 S3



CM 2

CRN 48028-76-8

CMF C2 H5 O4 S

Et-O-SO₃⁻

L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:18578 CAPLUS

DOCUMENT NUMBER: 45:18578

ORIGINAL REFERENCE NO.: 45:3273f-i,3274a-b

TITLE: Improvements in carbocyanine photographic sensitizing dyes

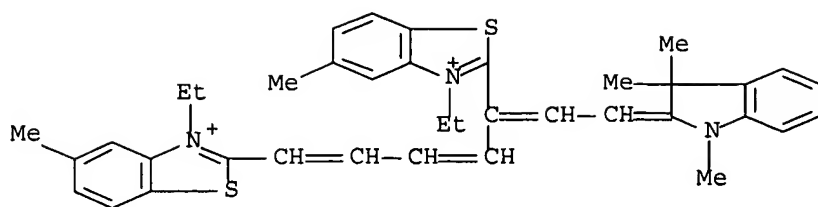
INVENTOR(S): Kendall, John D.; Doyle, Frank P.

PATENT ASSIGNEE(S): Ilford Ltd.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

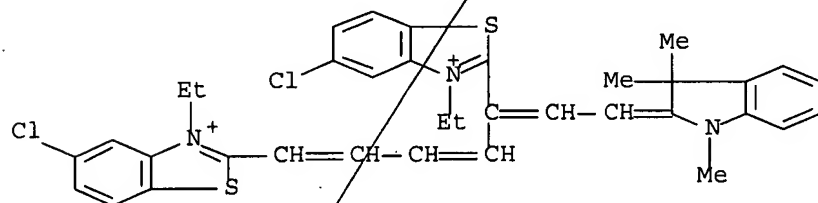
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	US 2534913		19501219	US 1948-30976	19480603
GI	For diagram(s), see printed CA Issue.				
AB	<p>Dye intermediates of the general type, D1.N(R)(A):(CH.CH)n:CCH:CHC(:CHSR'')C:(CH.CH)n:N(R')(X)D2, prepd. as described in Brit. 638,023 (cf. following abstr.), in which n is zero, D1 and D2 are the same or different and represent residues of 5-membered heterocyclic systems, R and R' are the same or different and are alkyl, hydroxyalkyl, aralkyl, or hydroxyaralkyl groups, R'' is an alkyl or aralkyl group, and A and X are acid radicals, are treated with solvolytic agents, e.g. H2O or an alc., to give photographic sensitizing dyes, D1.N(R).C:CHCH:C(CHO).C:N(R')(X)D2, or the isomer in which the -CHO is attached at the C atom nearer to the D1 ring. Isolation of the intermediates is not necessary. Reaction mixts. from the process, described in Brit. 638,023, contg. the required intermediate may be treated directly with the solvolytic reagent, reaction occurring either upon allowing the reagents to stand together or upon warming (as long as 30 min. may be required). 3,3'-Diethylthiacarbocyanine iodide 4.9 p-MeC6H4SO3H 2.5, HC(SET)3 2.5, and Ac2O 25 parts by wt. are refluxed until bright, yellow-orange (approx. 5 min.). Removing the solvent under reduced pressure, washing the residue with Et2O, dissolving in EtOH, and pouring into aq. KI soln. gives 3,3'-diethyl-8-formylthiacarbocyanine iodide, crystn. from MeOH, orange with a green reflex, m. 253.degree. (decompn.), also prepd. by use of 2.0 parts HC(SMe)3 or 4.0 parts (PhCH2S)3CH in place of HC(SET)3; in a gelatinous Ag iodobromide emulsion it imparts a sensitivity band extending to 5800 A., with a sharp max. at 5500 A. The following dyes are prepd. similarly: 3,3'-diethyl-8-formyl-4,5,4',5'-benzobenzoxacarbocyanine iodide, red crystals from MeOH, m. 278.degree. (decompn.); 3,3'-diethyl-8-formylselenocarbocyanine iodide, brown glistening crystals from MeOH, m. 256.degree. (decompn.), sensitivity band to 6000 A., max. about 5400 A.; 3,3'-diethyl-5,5'-dimethyl-8-formylthiacarbocyanine iodide, red-brown, crystals from MeOH, m. 265.degree. (decompn.), sensitivity band to 6000 A., max. about 5500 A.; 3,3'-diethyl-5,5'-dichloro-8-formyl-thiacarbocyanine iodide, brown powder, m. 298.degree. (decompn.); 3,3'-diethyl-4,5,4',5'-dibenzo-8-formylthiacarbocyanine iodide, brown needles from MeOH, m. 302.degree. (decompn.).</p>				
IT	<p>878787-03-2P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-methyl-iodide] 878787-04-3P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide RL: PREP (Preparation) (prepn. of)</p>				
RN	878787-03-2 CAPLUS				
CN	Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-methyl-iodide] (5CI) (CA INDEX NAME)				



● I⁻

RN 878787-04-3 CAPLUS

CN Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide (5CI) (CA INDEX NAME)



● I⁻

L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:18577 CAPLUS

DOCUMENT NUMBER: 45:18577

ORIGINAL REFERENCE NO.: 45:3273f-i,3274a-b

TITLE: Improvements in carbocyanine photographic sensitizing dyes

INVENTOR(S): Kendall, John D.; Doyle, Frank P.

PATENT ASSIGNEE(S): Ilford Ltd.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

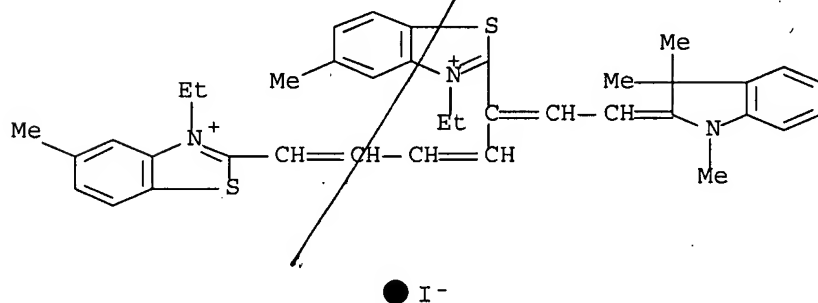
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 638022		19500531	GB 1947-14792	19470604

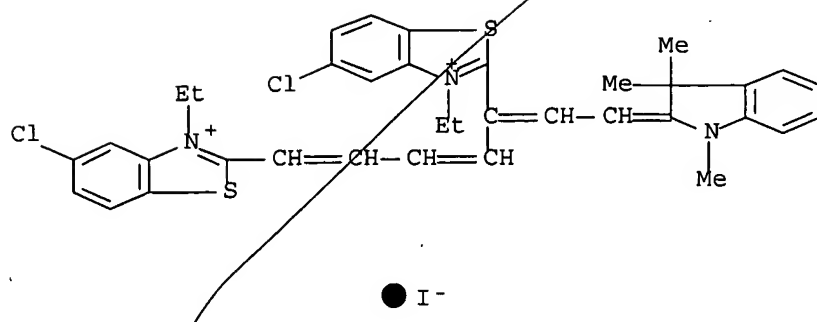
GI For diagram(s), see printed CA Issue.

AB Dye intermediates of the general type, D1.N(R)(A):(CH.CH)n:CCH:CHC(:CHSR')C:(CH.CH)n:N(R')(X)D2, prepd. as described in Brit. 638,023 (cf. following abstr.), in which n is zero, D1 and D2 are the same or different and represent residues of 5-membered heterocyclic systems, R and R' are the same or different and are alkyl, hydroxyalkyl, aralkyl, or hydroxyaralkyl groups, R' is an alkyl or aralkyl group, and A and X are acid radicals, are treated with solvolytic agents, e.g. H2O or an alc., to give photographic sensitizing dyes, D1.N(R).C:CHCH:C(CHO).C:N(R')(X)D2, or the isomer in which the -CHO is

IT 878787-03-2P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinyli-
dene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-methyl-
iodide] 878787-04-3P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-
trimethyl-2-indolinyli-
dene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-
ethyl-, iodide
RL: PREP (Preparation)
(prepn. of)
RN 878787-03-2 CAPLUS
CN Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinyli-
dene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-methyl- iodide] (5CI) (CA INDEX NAME)



RN 878787-04-3 CAPLUS
CN Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinyli-
dene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide (5CI) (CA INDEX NAME)



L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:15913 CAPLUS
 DOCUMENT NUMBER: 45:15913
 ORIGINAL REFERENCE NO.: 45:2803d-i,2804a
 TITLE: Cyanine dye intermediates
 INVENTOR(S): Kendall, John D.; Doyle, Frank P.
 PATENT ASSIGNEE(S): Ilford Ltd.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2533816		19501212	US 1948-30977	19480603

GI For diagram(s), see printed CA Issue.

AB Cyanine dye intermediates, used in the synthesis of trinuclear polymethine photographic emulsion sensitizers, are prep'd. from cyanine dyes and are believed to have the structure D'.N(R')(A):(CH.CH)n:C(CH:CH)xC(:CHSR''')C:(CH.CH)n:N(R'')(X).D'', where R' and R'' are alkyl, hydroxyalkyl, aralkyl, or hydroxyaralkyl groups, D' and D'' are residues of 5- or 6-membered heterocyclic nuclei, n is 0 or 1, x is 1 or 2, A and X are acid radicals, and R''' is an alkyl or aralkyl group. Thus, 1,1'-diethyl-2,2'-quinocarbocyanine iodide 4.8, p-toluenesulfonic acid 2.5, and triethyltrithio orthoformate 2.2 parts refluxed in acetic anhydride, the excess solvent removed by evapn. in vacuo, washed with Et₂O, dissolved in EtOH, poured into aq. KI soln., the filtered ppt. washed with H₂O followed by EtOH, and crystd. from EtOH yields orange-red needles of 1-(ethylmercapto)-2,4-di-2-quinolyl-1,3-butadiene di-EtI, m. 176.degree. (decompn.). The following dye intermediates were prep'd. in a similar manner: 1-(ethylmercapto)-2,4-bis(2-benzothiazolyl)-1,3-butadiene bis(Et p-toluenesulfonate), 1-(ethylmercapto)-2,4-bis(2-benzothiazolyl)-1,3-butadiene EtI Et p-toluenesulfonate (a hygroscopic yellow solid), 1-(methylmercapto)-2,4-bis(2-benzothiazolyl)-1,3-butadiene bis(Et p-toluenesulfonate), 1-(benzylmercapto)-2,4-bis(2-benzothiazolyl)-1,3-butadiene bis(Et p-toluenesulfonate), 1-(ethylmercapto)-2,4-bis(5-methyl-2-benzothiazolyl)-1,3-butadiene Et p-toluenesulfonate EtI 1-(ethylmercapto)-2,4-bis(5-methyl-2-benzothiazolyl)-1,3-butadiene di-EtI, m. 254.degree. (decompn.), 1-(ethylmercapto)-2,4-bis(5-chloro-2-benzothiazolyl)-1,3-butadiene bis(Et p-toluenesulfonate). 1-(ethylmercapto)-2,4-bis(5-chloro-2-benzothiazolyl)-1,3-butadiene di-EtI, m. 190.degree. (decompn.), 1-(ethylmercapto)-2,4-bis(4',5'-benzbenzothiazol-2-yl)-1,3-butadiene bis(Et p-toluenesulfonate), 1-(ethylmercapto)-2,4-bis(4',5'-benzbenzothiazol-2-yl)-1,3-butadiene di-EtI, 1-(benzylmercapto)-2,4-bis(4',5'-benzbenzothiazol-2-yl)-1,3-butadiene bis(Et p-toluenesulfonate), m. 80.degree. (decompn.), 1-

(ethylmercapto)-2,4-di-2-quinolyl-1,3-butadiene di-EtBr, 1-(ethylmercapto)-2,4-di-2-quinolyl-1,3-butadiene EtBr Et 2-naphthalenesulfonate, 1-(ethylmercapto)-2,4-di-4-quinolyl-1,3-butadiene EtBr Et p-toluenesulfonate, 1-(ethylmercapto)-2,4-di-4-quinolyl-1,3-butadiene di-EtI m. 283.degree. (decompn.), 1-(ethylmercapto)-2,4-di-2-benzoselenazolyl-1,3-butadiene bis(Et p-toluenesulfonate), 1-(ethylmercapto)-2,6-bis(3,3-dimethyl-3H-pseudoindolyl)-1,3,5-hexatriene MeI Me p-toluenesulfonate, 1-(ethylmercapto)-2,6-bis(5-methyl-2-benzothiazolyl)-1,3,5-hexatriene EtI Et p-toluenesulfonate, 1-(ethylmercapto)-2,6-bis(5-chloro-2-benzothiazolyl)-1,3,5-hexatriene EtI Et p-toluenesulfonate, and 1-(ethylmercapto)-2,4-di-2-benzothiazolyl-1,3-butadiene bis(Et p-toluenesulfonate).

IT 857395-00-7P, Pseudoindolium, 2,2'-[5-[(ethylthio)methylene]-1,3-pentadienylene]bis[1,3,3-trimethyl-3H-], iodide, p-toluenesulfonate
 RL: PREP (Préparation)
 (prepn. of)

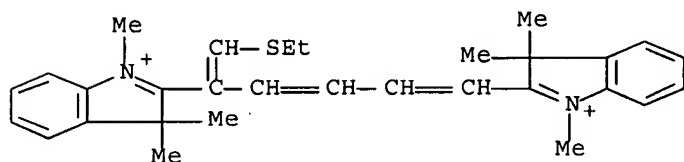
RN 857395-00-7 CAPLUS

CN Pseudoindolium, 2,2'-[5-[(ethylthio)methylene]-1,3-pentadienylene]bis[1,3,3-trimethyl-3H-], iodide, p-toluenesulfonate (5CI)
 (CA INDEX NAME)

CM 1

CRN 857394-99-1

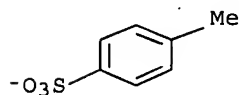
CMF C30 H36 N2 S



CM 2

CRN 16722-51-3

CMF C7 H7 O3 S



L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:7536 CAPLUS

DOCUMENT NUMBER: 45:7536

ORIGINAL REFERENCE NO.: 45:1350e-i,1351a-f

TITLE: Cyanine dyes

INVENTOR(S): Kendall, John D.; Doyle, Frank P.

PATENT ASSIGNEE(S): Ilford Ltd.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2518476		19500815	US	

AB 1-Ethylmercapto-2,4-dibenzothiazolyl-1,3-butadiene dietho-p- toluenesulfonate 2.7 and 2-methylbenzothiazole-EtI (I) 1.5 were heated in anhyd. C5H5N 20 parts for 10 min., the blue soln. was added to aq. KI, dild. with H2O, and cooled to give green bis-2-(3-ethylbenzothiazole)-.gamma.,2'-(3-ethylbenzothiazole)pentamethinecyanine diiodide, m. 247.degree. (from MeOH) (all m.ps. are with decompn.). Other products were similarly prepd. with corresponding intermediates and reagents such as I (read dye, color, m.p. and reagent). 2-(3-Ethylbenzothiazole)-2'-(1-ethylquinoline)-.gamma.,2'-(3-ethylbenzothiazole)pentamethinecyanine diiodide, green needles, 236.degree., quinaldine-EtI (II); 2'-(3-ethylbenzoxazole) analog, green, 190.degree., 2-methylbenzoxazole-EtI (III); 2'-(1,3,3-trimethylindolenine) analog, brassy green, 184.degree., 1,3,3-trimethyl-2-methyleneindolenine; bis-2-(3-ethyl-5-methylbenzothiazole)-.gamma.,2'-(3-ethyl-5-methylbenzothiazole)pentamethine cyanine diiodide, green, m. 248.degree., 2,5-dimethylbenzothiazole-EtI; 2-(3-ethyl-5-methylbenzothiazole)-2-(1,3,3-trimethylindolenine) analog, green, 192.degree., 1,3,3-trimethyl-2-methylenedihydroindolenine; bis-2-(3-ethyl-5-chlorobenzothiazole)-.gamma.,2'-(3-ethyl-5-chlorobenzothiazole)pentamethinecyanine diiodide, golden, 260.degree., 2-methyl-5-chlorobenzothiazole-EtI; bis-2-(1-ethylquinoline)-.gamma.,2'-(1-ethylquinoline)pentamethinecyanine diiodide, yellow-green, 236.degree., II; and bis-2-(3-ethylbenzoselenazole)-.gamma.,2'-(3-ethylbenzoselenazole)pentamethinecyanine monoiodide mono-p- toluenesulfonate, bright green, 245.degree., 2-methylbenzoselenazole-EtI. Tetramethine merocyanines were prepd. similarly: [2-(3-ethylbenzothiazole)-5'-(3-ethyl-2-thio-4-ketotetrahydrothiazole)-.gamma.,2'-(3-ethylbenzothiazole)tetramethinemerocyanine] iodide, green, 246.degree., 3-ethyl-2-thio-4-ketothiazolidene (IV); 5'-(3-methyl) analog, coppery green, 242.degree., 3-Me analog (V) of IV; 4'-(1-phenyl-3-methyl-5-pyrazolone) analog, green, 194.degree., 1-phenyl-3-methyl-5-pyrazolone (VI); [2-(3-ethyl-5-methylbenzothiazole)-5'-(3-methyl-2-thio-4-keto- tetrahydrothiazole)-.gamma.,2'-(3-ethyl-5-methylbenzothiazole)tetramethin emerocyanine] iodide, golden, 212.degree., V; 5'-(3-ethyl) analog, blue-green, 210.degree., IV; 4'-(1-phenyl-3-methyl-5-pyrazolone) analog, brown-green, 258.degree., VI; [2-(3-ethyl-5-chlorobenzothiazole)-5'-(3-methyl-2-thio-4-ketotetrahydrothiazole)-.gamma.,2'-(3-ethyl-5-chlorobenzothiazole)tetramethinemerocyanine] iodide, dark green, 210.degree., V; 5'-(3-ethyl) p-toluenesulfonate analog, yellow-green, 236.degree., IV; 4'-(1-phenyl-3-methyl-5-pyrazolone) analog, brassy green, 258.degree. (from C5H5N-MeOH), VI; [2-(3-ethyl-4,5-benzobenzothiazole)-5'-(3-ethyl-2-thio-4-keto-tetrahydrothiazole)-.gamma.,2'-(3-ethyl-4,5-benzobenzothiazole)tetramethinemerocyanine] iodide, magenta, 283.degree. (from C5H5N), IV; 5'-(3-methyl) p-toluenesulfonate analog, blue-green, 241.degree., V; 4'-(1-phenyl-3-methyl-5-pyrazolone) p-toluenesulfonate analog, green, 212.degree., VI; [2-(1-ethylquinoline)-5'-(3-ethyl-2-thio-4-ketotetrahydrothiazole)-.gamma.,2'-(1-ethylquinoline)tetramethinemerocyanine] iodide, dark green, 204.degree., IV; 5'-(3-methyl) bromide analog, light green, 210.degree., V; 4'-(1-phenyl-3-methyl-5-pyrazolone) analog, green, 260.degree., VI; 5'-(3-ethyl-2-thio-4-ketotetrahydrooxazole) analog, light green, 248.degree., 3-ethyl-2-thio-4-ketotetrahydrooxazole; [2-(3-ethylbenzoselenazole)-5'-(3-ethyl-2-thio-4-ketotetrahydrothiazole)-.gamma.,2'-(3-ethylbenzoselenazole)tetramethinemerocyanine] iodide, brown, 244.degree., IV; 5'-(3-methyl) analog, brassy green, 235.degree., V; 4'-(1-phenyl-3-methyl-5-pyrazolone) analog, shiny green, 193.degree., VI. A dye intermediate 13 parts (prepd. from bis-2-(1,3,3-trimethylindolenine)pentamethinecyanine iodide) was

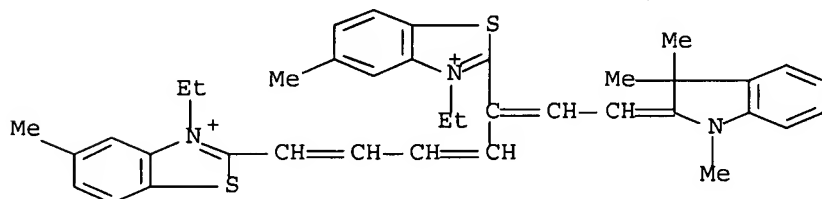
heated 5 min. with 2,3,3-trimethylindolenine-MeI (VII) 7.5 and Ac2O 400 parts, the cooled mixt. treated with Et2O, and the pptd. tar solidified by trituration in Me2CO and crystd. from MeOH to give brown cryst. bis-2-(1,3,3-trimethylindolenine)-.gamma.,2'-(1,3,3-trimethylindolenine)heptamethinecyanine diiodide, m. 238.degree.; 2-(3-ethylbenzothiazole) analog, dark brown, 214.degree., I; 2-(1-ethylquinoline) analog, dark blue, 213.degree., II; [5-(3-methyl-2-thio-4-ketotetrahydrothiazole)-2-(1,3,3-trimethylindolenine)-.beta.,2''-(1,3,3-trimethylindolenine)heptamethinemer ocyanine] iodide, royal blue, 209.degree., V (30 min. heating required); bis-2-(3-ethyl-5-methylbenzothiazole)-.gamma.,2'-(3-ethyl-5-methylbenzothiazole)heptamethinecyanine diiodide, dark blue, 213.degree., 1,6-dimethylbenzothiazole-EtI; 2-(1-ethylquinoline)-2'-(3-ethyl-5-methylbenzothiazole)-.gamma.,2''-(3-ethyl-5-methylbenzothiazole)heptamethinecyanine diiodide, green, 225.degree., II; 2-(1,3,3-trimethylindolenine) analog, dark green, 310.degree., VII; 2-(3-ethylbenzoxazole) analog, green, 222.degree., III; bis-2-(3-ethyl-5-chlorobenzothiazole)-.gamma.,2'-(3-ethyl-5-chlorobenzothiazole)heptamethinecyanine diiodide, green, 238.degree., 2-methyl-5-chlorobenzothiazole-EtI; 2-(1-ethylquinoline)-2'-(3-ethyl-5-chlorobenzothiazole)-.gamma.,2''-(3-ethyl-5-chlorobenzothiazole)heptamethinecyanine diiodide, dark green, 225.degree., II; and 2-(1,3,3-trimethylindolenine) analog, light blue, 214.degree., VII.

IT 878787-03-2P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinyldiene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-iodide] 878787-04-3P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinyldiene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide]

RL: PREP (Preparation)
(prepn. of)

RN 878787-03-2 CAPLUS

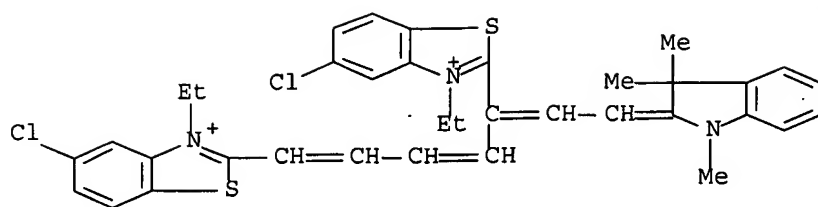
CN Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinyldiene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-iodide] (5CI) (CA INDEX NAME)



● I⁻

RN 878787-04-3 CAPLUS

CN Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinyldiene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide] (5CI) (CA INDEX NAME)



● I⁻

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	57.40	229.71
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.80	-7.80

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